1,4-Dioxane

123-91-1 | DTXSID4020533

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 13.2 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.26e-01

Confidence level: 5.78e-01

Nearest Neighbors from the Training Set

Image not found
1,4-Dioxane
Measured: 17.0
Predicted: 13.2

Image not found
2,2'-Bioxirane
Measured: 2.51
Predicted: 4.97

Image not found
Pyridine
Measured: 39.8
Predicted: 20.1

Image not found
1,2-Propylene glycol
Measured: 2.29
Predicted: 4.24

Image not found
Acrylamide
Measured: 50.1
Predicted: 16.7